

LISTING OF AND AMENDMENTS TO CLAIMS:

1. (currently amended) A method for obtaining at least one calibration filter for a Mass Spectrometry (MS) instrument system, comprising the step of:

obtaining, for a given calibration ~~standard~~ ion with its isotopes, measured isotope peak cluster data in a mass spectral range;

calculating, for the given calibration ~~standard~~ ion with its isotopes, relative isotope abundances and actual mass locations of isotopes corresponding thereto;

specifying mass spectral target peak shape functions;

performing convolution operations between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data; and

performing a deconvolution operation between the measured isotope peak cluster data and the calculated isotope peak cluster data after the convolution operations to obtain the at least one calibration filter.

2. (original) The method of claim 1, wherein any of said steps of performing convolution operations and performing a deconvolution operation employs at least one of a Fourier Transform, a matrix multiplication, and a matrix inversion.

3. (original) The method of claim 1, further comprising the step of pre-aligning measured mass spectral isotope peaks based on a least squares fit between centroid masses of the calculated relative isotope abundances and those of the measured isotope peak clusters, in a pre-calibration step performed subsequent to said calculating step.

4. (original) The method of claim 1, further comprising the steps of:

performing pre-calibration instrument-dependent transformations on raw mass spectral data; and

performing post-calibration instrument-dependent transformations on a calculated data set corresponding to a test sample.

5. (original) The method of claim 4, wherein said steps of performing pre-calibration instrument-dependent transformations and performing post-calibration instrument-dependent transformations involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero element along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration instrument-dependent transformations and the post-calibration instrument-dependent transformations, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

6. (original) The method of claim 5, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

7. (original) The method of claim 6, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and the raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

8. (original) The method of claim 7, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

9. (original) The method of claim 8, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

10. (original) The method of claim 7, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

11. (original) The method of claim 1, further comprising the steps of:
performing a pre-calibration mass spacing adjustment from a non-uniformly spaced mass acquisition interval to a uniformly spaced mass interval; and
performing a post-calibration mass spacing adjustment from the uniformly spaced mass interval to a reporting interval.

12. (original) The method of claim 11, wherein said steps of performing the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero element along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

13. (original) The method of claim 12, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

14. (original) The method of claim 13, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

15. (original) The method of claim 14, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

16. (original) The method of claim 15, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

17. (original) The method of claim 14, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

18. (original) The method of claim 1, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

19. (original) The method of claim 18, wherein said interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes the at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

20. (original) The method of claim 19, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

21. (currently amended) The method of claim 1, further comprising the step of introducing ~~adding~~ the calibration standard ~~into a test sample~~ one of prior to and in real-time through at least one of continuous infusion and online mixing so as to acquire both calibration data and test data in a single ~~mass spectral acquisition~~ experiment.

22. (currently amended) A method of processing raw mass spectral data, comprising the steps of:

applying a total filtering matrix to the raw mass spectral data to obtain calibrated mass spectral data,

wherein the total filtering matrix is formed by:

measured isotope peak cluster data, obtained for a given calibration ~~standard~~ ion in a mass spectral range

relative isotope abundances and actual mass locations of isotopes corresponding thereto, calculated for a same calibration ~~standard~~ ion,

specified mass spectral target peak shape functions,

convolution operations performed between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data; and

a deconvolution operation performed between the measured isotope peak cluster data and calculated isotope peak cluster data after the convolution operations to obtain at least one calibration filter for the total filtering matrix.

23. (original) The method of claim 22, wherein said applying step further comprises the step of interpolating the raw mass spectral data onto a same mass axis as that required by the total filtering matrix.

24. (original) The method of claim 22, wherein said applying step further comprises the step of interpolating the calibrated mass spectral data onto any desired mass axis different from that given by the total filtering matrix.

25. (original) The method of claim 22, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

26. (original) The method of claim 25, wherein weights of the weighted regression operation are proportional to an inverse of mass spectral variances.

27. (original) The method of claim 22, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

28. (currently amended) A method for analyzing peaks corresponding to data obtained from an instrument system used for performing at least one of separation and analysis of analytes, the method comprising the steps of:

applying a weighted regression operation to peaks within a range; and
reporting regression coefficients as one of integrated peak areas, ~~peak positions,~~
and peak position deviations ~~corresponding to one of nominal peak position and~~
~~estimated actual peak position.~~

29. (currently amended) The method of claim 28, wherein said method is performed subsequent to the instrument system being calibrated such that peak shape functions are given by target peak shape functions to form the basis of said regression operation.

30. (original) The method of claim 28, wherein weights of the weighted regression operation are proportional to an inverse of peak intensity variances.

31. (currently amended) The method of claim 28, wherein said applying and reporting steps are repeated until incremental improvements in at least one of the integrated peak areas, peak positions and the peak position deviations meet preset criteria.

32. (currently amended) The method of claim 28, wherein said analyzing step further comprises the step of calculating standard deviations for one of the integrated peak areas, peak positions, and the peak position deviations based on ~~weights~~ of the weighted regression.

33. (currently amended) The method of claim 32, wherein said calculating step further comprises the step of calculating t-statistics for at least one of the integrated peak areas, peak positions, and the peak position deviations, the t-statistics being adapted for testing and reporting a statistical significance of at least one of calculated peak areas and peak locations, wherein the statistical significance indicates a presence or an absence of a peak.

34. (original) The method of claim 28, further comprising the step of creating a peak component matrix, including calculating a pair of matrix rows, with a first row of the pair of matrix rows for storing a peak shape function and with a second row of the pair of matrix rows for storing a first derivative of the peak shape function stored in the first row.

35. (original) The method of claim 34, wherein the peak shape function includes additionally at least one of linear and nonlinear functions to account for baseline components.

36. (original) The method of claim 34, wherein the peak shape function is one of target peak shape function and a known instrument peak shape function.

37. (original) The method of claim 36, wherein the peak shape function and the first derivative thereof are identical across a range and are both sampled at a same integer fraction of a nominal peak spacing.

38. (original) The method of claim 37, further comprising the step of completing the peak component matrix such that any peak shape functions in any remaining matrix rows are arranged as shifted versions of each other corresponding to each nominal position within a range of positions.

39. (currently amended) The method of claim 34, further comprising one of:
updating nominal positions in the peak component matrix to estimated actual positions by adding reported deviations to the nominal positions; and
updating the estimated actual positions in the peak component matrix to further refined estimated actual positions by adding reported deviations to the estimated actual positions.

40. (currently amended) The method of claim 28, further comprising the step of one of calculating and interpolating data corresponding to peak shape functions to obtain one other peak shape function at each of the nominal positions.

41. (original) The method of claim 40, wherein said interpolating step comprises the steps of:
collecting the peak shape functions as vectors in a matrix for decomposition;
decomposing the peak shape functions included in the matrix;
interpolating between decomposed vectors to obtain interpolated vectors; and
reconstructing the one other peak shape function at each of the nominal positions using the interpolated vectors.

42. (original) The method of claim 41, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

43. (original) The method of claim 40, further comprising the step of calculating first derivatives of the peak shape functions at each of the nominal positions.

44. (original) The method of claim 43, further comprising the step of creating a peak component matrix, by combining the peak shape functions and the first derivatives corresponding thereto.

45. (currently amended) The method of claim 44, further comprising one of:
updating nominal positions in the peak component matrix to estimated actual positions by adding reported deviations to the nominal positions; and
updating the estimated actual positions in the peak component matrix to further refined estimated actual positions by adding reported deviations to the estimated actual positions.

46. (original) The method of claim 44, wherein the peak component matrix includes additionally at least one of linear and nonlinear functions to account for baseline components.

47. (original) The method of claim 28, wherein said applying step further comprises the step of performing at least one of a matrix inversion and a matrix decomposition.

48. (original) The method of claim 47, wherein the at least one of the matrix inversion and the matrix decomposition is based on at least one of a banded nature, a symmetrical nature, and a cyclic nature of a peak component matrix.

49. (original) The method of claim 47, wherein results of at least one of the matrix inversion and the matrix decomposition are calculated and stored prior to analyzing test sample data.

50. (currently amended) The method of ~~any one of claims~~ claim 28 ~~to 49~~, wherein said instrument system includes at least one of a mass spectrometer and separation apparatus, and said position within a range corresponds to a mass location.

51. (currently amended) The method of ~~any one of claims~~ claim 28 ~~to 49~~, wherein said instrument system includes at least one of a liquid chromatograph and a gas chromatograph, and said position within a range corresponds to time of occurrence of a peak.

52. (currently amended) The method of ~~any one of claims~~ claim 28 ~~to 49~~, wherein said instrument system includes a spectroscopy system, and said position within a range corresponds to one of frequency, shift, and wavelength.

53. – 109. (canceled)

110. (currently amended) For use in a mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, a computer readable medium having placed thereon computer readable program instructions for performing the method of claims ~~of any one of claims~~ 1 – 27, ~~53 – 103, 105 – 108, or 114.~~

111. (currently amended) For use in an instrument system having associated therewith a computer for performing data analysis functions of data produced by the instrument system, a computer readable medium having placed thereon computer readable program instructions for performing the method of claims ~~of any one of claims~~ 28 – 49, ~~91 – 108, or 114.~~

112. (currently amended) A mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, the computer performing the method of ~~any one of claims~~ 1 – 27, ~~53 – 103, 105 – 108, or 114.~~

113. (currently amended) An instrument system having associated therewith a computer for performing data analysis functions of data produced by the instrument

system, the computer performing the method of ~~any one of claims 28 — 49, 91 — 108, or~~
114.

114. (currently amended) The method of claim 1 ~~or claim 53~~, wherein said calibration filter, when applied to a mass spectrum, performs at least one of noise filtering, signal averaging, mass calibration, and peak shape adjustment.

115. (new) For use in a mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, a computer readable medium having placed thereon computer readable program instructions for performing the method of claim 22.

116. (new) A mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, the computer performing the method of claim 22.